ULTRAFAST SPECTROSCOPIC AND *AB INITIO* COMPUTATIONAL INVESTIGATIONS ON SOLVATION DYNAMICS OF NEUTRAL AND DEPROTONATED TYROSINE.

TAKASHIGE FUJIWARA, *Center for Photochemical Sciences, Bowling Green State University, Bowling Green, OH, USA*; MAREK Z. ZGIERSKI, *Steacie Laboratory, National Research Council of Canada, Ottawa, ON, Canada*.

We have studied one of the aromatic amino acids, tyrosine, regarding its photophysical properties in various solvent conditions by using a femtosecond fluorescence up-conversion technique and high-level TDDFT and CC2 computations. In this talk, profound details not only on ultrafast solvation dynamics on a neutral tyrosine in various solvents, but also on the excited-state dynamics for a single- (or doubly-) deprotonated tyrosine under various pH solutions will be presented. In high basicity, a tyrosine shows different absorption/emission spectra, and a total spectrum consists of a combination of these individual spectra that depend on the pH of the solution. The time scale of acid–base equilibrium is essential in solvation dynamics; whereas the protonation is simply controlled by diffusion, the de-protonation is considered to be slow process such that acid–base equilibrium may not be reached in the short-lived excited state after photo-excitation. Experimental and computational approaches taken and insights obtained in this concerted work will be described.